MST*e* NEWS

INSIDE

Rafael Spillers sets up a scanning electron microscope in the Materials Science Laboratory. As a research technician for MST-16, Spillers performs actinide materials science to support the Lab's national security science mission.
Photo by Sandra Valdez, XIT-TSS

"

[The Lab] represents so many different cultures and ways of thinking ...There are a lot of cool things here that excite me, and a lot of imagination. It's been amazing so far. *"*

Rafael Spillers

*Discovering impurities,
one element at a time*

By Kris Fronzak, ADEPS Communications

After a childhood shaped by government initiatives that improve opportunities for struggling families, Rafael Spillers said he saw the Laboratory as an ideal way to give back.

"[In the United States], if you apply yourself the government has set it up in such a way that there are opportunities to pull yourself out. So to take my knowledge and skill set and give back to my government is an honor."

Spillers grew up in southern New Mexico with his mom and brother. A newspaper classified ad that read "Wanted: SEM operator. Willing to train" was all it took for him to enter to the world of microscopy, fresh out of high school. The company behind the advertisement, Analytical Solutions, has scanning electron microscopy (SEM), mechanical, and metallurgical lab capabilities. Spillers credits it not only for launching his career, which spans more than 20 years, but

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From David's desk . . .

> *[The Lab] represents so many different cultures and ways of thinking,...There are a lot of cool things here that excite me, and a lot of imagination. It's been amazing so far.*

I'd like to welcome everyone back from the holiday break after relaxing and enjoying the time with family and friends. As we return to work I hope that we are refreshed and ready to tackle the new challenges in 2017.

Change seemed to be a theme in 2016 with the MST/Sigma Division reorganization and MST group management changes as well as changes on the national level. Although that change could be a distraction, MST Division achieved great success meeting mission deliverables and milestones and producing a high-level of peer-reviewed publication output. I'd like to thank all of you for your hard work over the last year demonstrating the value of MST Division to our mission customers through our exceptional materials science and technology. We have also aggressively hired in 2016 to both replenish and strengthen our workforce with the addition of 20 new regular staff (technicians and scientists/engineers)—and we are projecting another 25 hires in 2017. With that comes a responsibility that we all share as we mentor and train this new workforce for successful integration into the Laboratory and MST Division.

As I look forward to 2017, I see a number of exciting challenges and opportunities for MST Division to continue having impact on a national level for our mission customers. Within the nuclear weapons program, plutonium aging has an increased level of attention and MST is taking a leadership role in reassessing our understanding of how plutonium ages and its potential impact on the stockpile. This increased level of interest is likely to rejuvenate an experimental and modeling aging program in MST to answer some of the outstanding questions. Continuing along the aging theme, many of our aging issues in weapons are polymer related, and our existing understanding and predictive capability is empirical at best. MST-7 and T Division have partnered to develop an experimental-modeling capability to improve our ability to predict polymer lifetimes. MST Division will continue to solve challenges in the B61 LEP and W88 refresh, in particular some of our efforts focused on process-structure-property-performance relationships associated with detonator qualification and insensitive high explosive manufacturing.

MST is also looking to expand its role in materials science in support of our nuclear energy programs. Expanding upon the capabilities in MST-7 and MST-8, we are assessing the establishment of an intermediate-scale fuel fabrication capability to synthesize prototype production quantities of new nuclear fuel forms to support early reactor testing of new fuels. In addition to complementing the nuclear fuel efforts in MST Division, this will support the Laboratory's priorities in micro and small modular reactor design and development.

Another opportunity for MST Division is in the development of next-generation detector materials. Leveraging our strengths in single crystal growth and materials design through modeling and machine learning, we will be embarking on a new detector material development initiative to support a number of Laboratory missions including nonproliferation, radiographic facilities (e.g. DARHT [Dual Axis Radiographic Hydrodynamic Test Facility] and Nevada) and accelerator technologies such as MaRIE (Matter Radiation Interactions in Extremes).

At the DOE level, there is interest in pursuing a cross-department initiative in materials for harsh environments. Materials in harsh environments is a common theme spanning multiple offices: next-generation heat exchangers for fossil energy, advanced nuclear fuel and pressure vessels, waste heat recovery systems, and advanced turbine technology. MST Division has a number of capabilities developed for our nuclear energy programs that could be applied to these broader technology problems. I have been working with a number of other national laboratories and federal program managers to define a future program. Be prepared to engage in this initiative sometime this year.

Desk cont.

Lastly, we have received capability development funding from PADSTE to reconfigure laboratories in the Materials Science Laboratory to support these and other future missions (e.g. production science), while also providing training opportunities for our new, uncleared workforce. We have been developing this in partnership with MPA, Sigma, and MET to develop their workforce as well.

2017 will be an exciting year as we tackle these new challenges and I look forward to working with all of you.

MST Division Leader David Teter

Spillers cont.

also for defining his work ethic. One of his Analytical Solutions mentors, Michael Strizich, advised Spillers to develop a system for whatever he did. That advice has stuck with him to this day.

"Those simple words anchored to my brain. I apply them to everything that I do at the lab and probably in my personal life. I was still driven before that, but not sure where to drive to," Spillers said.

Work at Analytical Solutions, Emcore, and a few other laboratories ultimately brought Spillers to the Laboratory, where he recently joined Nuclear Materials Science (MST-16) as a research technician supporting its mission of performing actinide materials science in support of national security. He will eventually become a metallographer for the group.

His advisor and team leader Terry Holesinger (MST-16) had nothing but accolades for his new mentoree.

"Rafael is a homegrown product, and I don't know if you'll meet a more enthusiastic employee. This is, to him, a dream job location," Holesinger said.

"[The Lab] represents so many different cultures and ways of thinking," Spillers agreed. "There are a lot of cool things here that excite me, and a lot of imagination. It's been amazing so far."

As a research technician, Spillers is performing scanning electron microscopy for the Santa Fe-based company iBeam. The business is developing and refining flexible light emitting diodes (LEDs) on gallium nitride films for use in the semiconductor industry, and for electronic components. The failure rate for these films is high, as foreign particles can be introduced in countless ways during the manufacturing process. Spiller's role involves tracking down errant particles, then investigating their shape, morphology, and elemental composition.

"It's kind of a failure analysis plus forensic investigation," Spillers said. "Eventually, we can figure out what about the particle is making these flexible LEDs fail, and then engineer them not to fail."

Spillers hailed the Lab's combination of resources and an emphasis on learning for allowing him to grow on the job. "Los Alamos does a really great job of allowing you to utilize your own expertise coupled with their resources, which opens up new doors and new discoveries," he said. "It's a very powerful Laboratory."

Rafael Spillers dream experiment

If Rafael Spillers could devise his ideal career, he would buy his own instruments and use them to conduct microscopic analyses of how things are put together. This knowledge would be an especially eye-opening educational tool for children, he said. "Say you cross section a human tooth—you'd see the dentin at the inner core, then you start seeing the outer portions. Wouldn't it be great if you could show kids that, and they could hold it in their hands? There's so much to be gained from that kind of looking." He also waxed scientific on what a bug's exoskeleton might look like or a CD that was burned versus blank.

But his favorite cross section? Human hair. Spillers took his own, set it in epoxy, and was surprised by the composition. "Most people don't really know how human hair is constructed. It looks cylindrical but can be flatter if it's closer to the root, and it has cracks radiating from the center," he explained. Spillers emphasized varied applications for this kind of research. So-called hair booms were even proposed to clean up oil after the Deepwater Horizon spill. He postulated that hair is a good tool because it is hollow and has cracks, so capillary action could soak up oils.

When you look at it that way, the real-world applications for creative cross sectioning are boundless.

MST staff in the news

Ghanshyam Pilania awarded Humboldt research Fellowship

Ghanshyam Pilania (Materials Science in Radiation and Dynamics Extremes, MST-8) has been chosen for a Humboldt Research Fellowship for Postdoctoral Researchers from the Alexander von Humboldt Foundation.

As a part of the fellowship, Pilania will visit the Fritz Haber Institute of the Max Planck Society in Berlin for 12 months, studying rational materials design using state-of-the-art materials informatics and data mining techniques. At the institute, he will develop materials informatics models for complex functional oxides with a particular focus on perovskites and related compounds. These models are of practical interest for a range of applications requiring materials with pre-specified functionalities, including scintillation, photovoltaics, electronic device applications, energy storage, and catalysis.

Pilania received his PhD in materials science and engineering from the University of Connecticut, where he focused on modeling of ferroelectric and catalytic properties of complex oxides using electronic structure theory. He was the recipient of the University of Connecticut's Materials Science and Engineering Department Outstanding Graduate Student Award.

He joined MST-8 as a postdoctoral research fellow in 2013 and was awarded a Director's Postdoctoral Fellowship in 2014. His postdoctoral research has largely focused on the development and application of materials modeling tools ranging from electronic- to atomic- to meso-scale, as well as simulations and materials informatics to understand and identify the relationships between the atomic scale structures/processes and the macroscopic behavior and properties of materials. He has authored or co-authored 44 publications in peer-reviewed journals.

The Humboldt foundation grants about 500 fellowships each year to highly qualified researchers who are starting their academic careers. The postdoctoral program allows recipients to spend 6-24 months in Germany on a research program of their choosing. Fellowships are granted on the basis of an applicant's academic record and performance, the quality of key publications, the originality and innovation potential of the suggested research, and the applicant's future academic potential.

Technical contact: Ghanshyam Pilania

Chris Stanek receives Laboratory's Fellows Prize in leadership

Chris Stanek (Materials Science in Radiation and Dynamics Extremes, MST-8) is a recipient of the Laboratory's Fellows Prize in leadership in science and engineering. The award commends individuals for outstanding scientific and engineering leadership at the Laboratory and recognizes the value of such leadership that stimulates the interest of young staff members in developing new technology.

Stanek maintained and enhanced the Lab's involvement in the Consortium for the Advanced Simulation of Light Water Reactors (CASL), and succeeded in turning the Fuels, Materials, and Chemistry focus area of CASL into a strong performer. Then Secretary of Energy Ernest Moniz said CASL is the most successful of the energy innovation hubs; this success is due to his efforts. Stanek is now the national technical director of Nuclear Energy's Nuclear Energy Advanced Modeling and Simulation (NEAMS). His work has been a boost for the Lab's reputation.

Dana Dattelbaum (Explosive Science and Shock Physics, M-DO) also received a Fellows Prize in leadership. Marc Janoschek, (Condensed Matter and Magnet Science, MPA-CMMS), Jennifer Martinez (Center for Integrated Nanotechnologies, MPA-CINT), and Jian-Xin Zhu (Physics of Condensed Matter and Complex Systems, T-4) were awarded the Fellows Prize in science and engineering.

"These scientists are being recognized for mission-relevant research and leadership that maintain the Lab's long-standing reputation for innovative scientific discoveries," said Chuck Farrar, the Engineering Institute Leader at the Laboratory's National Security Education Center and the coordinator of the Fellows Organization. "I congratulate all of them on their achievements."

Technical contact: Chris Stanek

'Virtual reactor' software wins R&D 100 Award

Capability relies on Los Alamos's advanced modeling and simulation expertise

An innovative capability for nuclear power, developed in part at Los Alamos National Laboratory (LANL), has been recognized with a 2016 R&D 100 Award. Virtual Environment for Reactor Applications (VERA) provides coupled, high fidelity software capabilities to examine light water reactors' operational and safety performance-defining phenomena at levels of detail previously unattainable. Chris Stanek (Materials Science In Radiation and Dynamics Extremes, MST-8) led the LANL team's efforts, which leveraged Los Alamos's experience in structure-property relations, mechanical deformation, and chemical kinetics in order to address several key aspects of nuclear fuel performance.

The R&D 100 Awards, often called the "Oscars of Innovation," are given by *R&D Magazine* to recognize the best technology products of the year.

VERA is a multiphysics simulation toolkit that enables users to study, mitigate, and manage problems identified by the nuclear power industry to a level of understanding not available through other toolsets. It supports options for both high-performance computing and industry-sized computing clusters in a manner that is accessible and easily understood for most users.

Oak Ridge National Laboratory submitted VERA, a joint entry with Core Physics, Electric Power Research Institute, Idaho National Laboratory, Los Alamos National Laboratory, Sandia National Laboratories, North Carolina State University, University of Michigan, and Westinghouse Electric Co. VERA was funded by the Consortium for Advanced Simulation of Light Water Reactors, a DOE Energy Innovation Hub.

"These awards are representative of the multidisciplinary character of the work we do at Los Alamos, and result from partnerships with other national laboratories, private industry, and universities," said Director Charlie McMillan. "I applaud all of the R&D 100 Award winners for their success and for showcasing the innovative science and technology that Los Alamos is known for."

The Laboratory also received R&D 100 Awards for Carbon Capture Simulation Initiative Toolset, PathScan, the Pulmonary Lung Model, and Entropy Engine. The Green Technology Special Recognition Award went to Turning Windows and Building Facades into Energy-Producing Solar Panels.

Since 1978, Los Alamos has won 137 of the prestigious R&D 100 Awards. The Laboratory's discoveries, developments, advancements, and inventions make the world a better and safer place, bolster national security, and enhance national competitiveness.

Technical contact: Chris Stanek

From left, MST Division Leader David Teter, Director for Civilian Nuclear Programs DV Rao, and Laboratory Director Charlie McMillan discuss the innovations behind VERA, "virtual reactor" software for nuclear power applications.

Pyrolytic carbon-coated fuel microspheres for self-regulating nuclear reactors

A compact nuclear reactor design capable of self-regulation is being developed as part of a Laboratory Directed Research and Development Directed Research (LDRD-DR) project. Self-regulating reactors are attractive because they can match varying operational needs while protecting the reactor core from exceeding thermal limits during abnormal events. This power source is ideal for unattended operations, and for applications in space and in remote areas. One of the promising directions in the development of advanced nuclear fuel forms is a transition from traditional single-phase fuels to composites consisting of fissile and non-fissile phases.

Los Alamos researchers have reestablished a fuel kernel coating technology last used decades ago that enables this development.

A Los Alamos nuclear fuel design team (Systems Design and Analysis, NEN-5) proposed a composite fuel constructed of closely packed pyrolytic carbon- (PyC) coated low-enriched uranium carbide (UC) kernels embedded in a graphite matrix (see Figure 1). The main purpose of the PyC layer in this design is to act as a thermal barrier to control heat release from a kernel into the matrix. During steady state operation the kernel and the matrix are in thermal equilibrium. If the coating performs according to the design, it will retain heat in the kernel during a reactivity spike. Therefore, high

fuel kernel temperatures trigger strong negative feedback by absorption of thermal and epithermal neutrons, mitigating an accident. The timing of the self-regulation feedback is controlled by the heat release from the kernel to the matrix, which is related to the PyC layer thickness, microstructure, and the two interfaces separating the kernel from the matrix (see Figure 2).

One of the most challenging aspects of this concept is the PyC coating, with finely tuned and anisotropic thermal transport impedance, which controls heat release from fuel kernels to the fuel matrix. Expertise in this coating technology disappeared from U.S. industry decades ago, but has now been reestablished within the MST Division. A unique capability for fabrication of such coatings on low-enriched UC kernels was set up in Engineered Materials (MST-7). Through collaboration with Manufacturing Engineering and Technology (MET-DO), Advanced Nuclear Technology (NEN-2), Sigma Division (Sigma-DO), Materials Science in Radiation and Dynamics Extremes (MST-8), and Nuclear Materials Science (MST-16), the fluidized bed chemical vapor deposition technology (FBCVD) used at LANL in the 1960s was rebuilt and brought up to current safety and efficiency standards. In addition, modern characterization tools (such as x-ray computed tomography) were applied to evaluate the properties of coated kernels. The Thin Films and Coatings team within MST-7 optimized FBCVD conditions to produce ~1.5 kg of PyC-coated fuel surrogate kernels of ZrO_2, HfO_2, and WC, as well as ~0.3 kg of naturally enriched UC kernels.
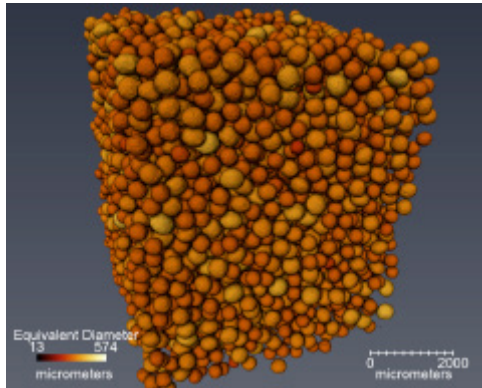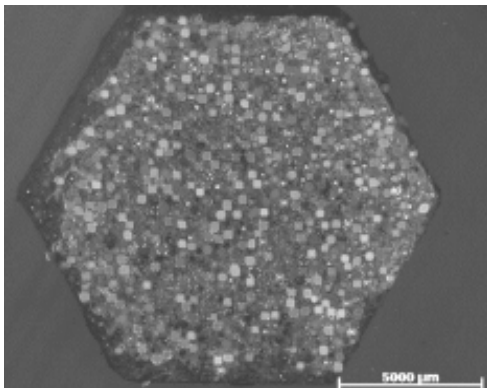
Figure 1, above: optical cross-sectional (left) and 3D x-ray computed tomography (right) images of an extruded graphite composite nuclear fuel rod surrogate with high loading (estimated 44 vol%) of PyC-coated spherical ZrO_2 kernels. The graphite matrix represents the non-fissile phase and PyC-coated ZrO_2 is a surrogate for the fissile (low-enriched UC) phase of the composite nuclear fuel concept.

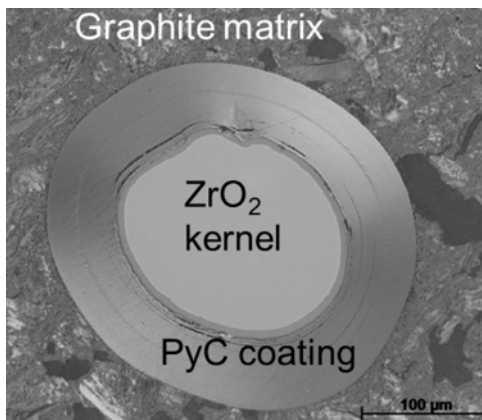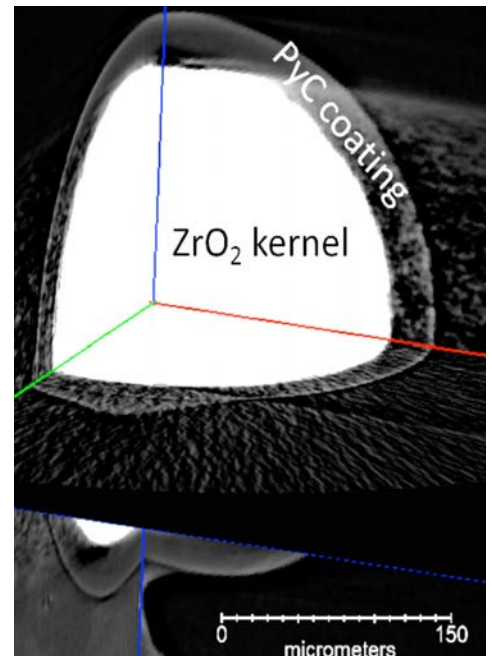**Figure 2, below: optical cross-sectional (left) and 3D x-ray computed tomography (right) images of a PyC-coated spherical ZrO_2 kernel embedded in a graphite matrix and without matrix, respectively.**

MST-16 contributes to understanding plutonium aging
Groups's research combination is one-of-kind in the DOE complex

Nuclear Materials Science (MST-16) plays a critical role in evaluating the static and dynamic properties of new and aged plutonium. The group's recent work, in collaboration with Shock and Detonation Physics (M-9), Materials Science in Radiation and Dynamics Extremes (MST-8), Condensed Matter and Magnet Science (MPA-CMMS), and Weapon Component Manufacturing and Surveillance (NCO-1), was an integrated effort to support the B61 Life Extension Program through the National Nuclear Security Administration's Science Program.

This effort started several years ago with casting simulation and mold development, plutonium casting, and thermal processing, machining, and small-sample preparation. This new cast material, along with aged plutonium samples, was characterized microstructurally using metallography and electron microprobe analysis. Individual sample density was determined using the immersion method and a new gas pycnometry capability. Elastic constants and sample quality were evaluated using resonant ultrasound spectroscopy. Once the characteristics of individual samples were known, mechanical and dynamic properties were measured using variable temperature resonant ultrasound spectroscopy, quasi-static compression testing, Kolsky bar testing, and 40-mm gas and powder shots. Several samples were prepared, assembled, and shipped to the Z Facility at Sandia National Laboratories for very high-strain rate testing. This combination of plutonium structure, properties, and performance research is unique in the DOE complex.

Technical contact: Jeremy Mitchell

MST-16 research technicians Ben Hollowell (near right) and Todd Martinez (far right) work on the PF-4 40-mm gun. The 40-mm gun is a key research tool for understanding the dynamic properties of plutonium.

Pyrolytic cont.

This LDRD-DR, "Multi-Scale Kinetics of Self-Regulating Nuclear Reactors" (Principal Investigator DV Rao), supports the Lab's Energy Security mission and its Materials for the Future science pillar.

Researchers: Miles Beaux, Kevin Hubbard, Brian Patterson, Kevin Henderson, Bryan Bennett, Douglas Vodnik, Reuben Peterson, and Igor Usov (MST-7); Erik Luther and Eric Tegtmeier (Sigma-DO); Graham King (MST-8); Alice Smith (MST-16); Jeffrey Goettee (NEN-2); and James Jurney (MET-DO).

Technical contact: Igor Usov

Celebrating service

Congratulations to the following MST Division employees recently celebrating service anniversaries:

Scott Richmond, MST-16. 30 years
Franz Freibert, MST-16 . . . . 20 years
Isaac Herrera, MST-7 . . . . 20 years
Deeann Chavez, MST-16 . . . . 15 years
David Pugmire, MST-16 . . . . 15 years
Joseph Reynolds, MST-16 . . . . 15 years
Fritzgerald Sandoval, MST-16. . . . . 15 years
Miles Beaux, MST-7 . . . . 5 years

Heads**UP!**

Taking action to protect the environment
LANL's Environmental Management System

The Laboratory has 12 Governing Policies for executing work, accomplishing mission, and providing management and oversight. The Governing Policy on the Environment ensures that all work is performed in a way that protects the environment.

As stewards of our environment and to achieve our mission in accordance with all applicable environmental requirements, we set continual environmental improvement objectives and targets using an Environmental Management System (EMS). An EMS is a set of processes and practices that enable an organization to protect the environment, prevent or mitigate adverse impacts, assure compliance, improve performance, communicate with interested parties, and provide management with the information needed to make effective environmental decisions. The Lab's EMS is certified to ISO 14001, which is an internationally recognized environmental management standard.

Every year, each directorate evaluates its activities and sets new environmental goals. These goals are documented in directorate-level environmental action plans. In MST, our goals are included in the ADEPS action plan.

Actions for this year include some goals from the past as well as new goals:
- Review of our chemical inventory to develop a proposal for disposal of unneeded chemicals > 10 years old;
- Identify all remaining SF_6 sources to determine if a path forward exists to either eliminate or reclaim SF_6;
- Acknowledge pollution prevention, recycling, etc., activities of employees;
- Communicate EMS information in posters, newsletters, division meetings, etc.;
- Support disposition and cleanup of legacy equipment;
- Support the implementation of LED lighting;
- Evaluate storm water monitoring requirements at Sigma; and
- Continue to work with the Lab's Environmental Sustainability Program Smart Lab initiative at MSL and TFF.

If you have any questions concerning our EMS, please contact Dianne Wilburn, dianne@lanl.gov. More information can also be found on the Laboratory's EMS website: int.lanl.gov/environment/ems/.

Highlights from 2016, clockwise from top: At TA-3, Building 34, we completed packaging some of the equipment from the basement as low level waste. This effort is ongoing. More than a dozen gloveboxes were recycled from the Sigma complex. Covered bins were put in place for storm water permit compliance. Chemical cabinets from Sigma were salvaged.

MST*e*NEWS
Materials Science and Technology

Published by the Experimental Physical Sciences Directorate.

To submit news items or for more information, contact Karen Kippen, ADEPS Communications, at 505-606-1822, or adeps-comm@lanl.gov.

For past issues, see www.lanl.gov/org/padste/adeps/mst-e-news.php.

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NNSA
National Nuclear Security Administration

LA-UR-17-21221

Title: MST e-News February 2017

Author(s): Kippen, Karen Elizabeth

Intended for: Newsletter
Web

Issued: 2017-02-16